The phylo4 S4 classes and methods

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1 Introduction

This document describes the new phylo4 S4 classes and methods, which are intended to provide a unifying standard for phylogenetic data in R. The base phylo4 class is modeled on the the phylo class in ape. phylo4d and multiphylo4 extend the phylo4 class to include data or multiple tree respectively. In addition to describing the classes and methods this vignette gives examples of how they might be used.

2 Package Overview

The phylobase package currently implements functions and data structures that implement the following:

- Data structures for storing a tree and multiple trees
- A data structure for storing a tree with associated tip and node data
- A data structure for storing multiple trees with one set of tip data
- Functions for reading nexus files into the above data structures
- Functions for converting between the above data structures and ape phylo objects as well as ade4 phylog objects
- Functions for subsetting, replacing, and plotting the above structures

3 Trees without data

You can start with a tree — an object of class phylo from the ape package (e.g., read in using the read.tree() or read.nexus() functions), and convert it to a phylo4 object.

For example, get the *Geospiza* data from the geiger package:

```
> library(geiger)
> data(geospiza)
> names(geospiza)

[1] "geospiza.tree" "geospiza.data"

    Convert the S3 tree to a S4 phylo4 object using the as() function:
> library(phylobase)
> g1 <- as(geospiza$geospiza.tree, "phylo4")
> g1

Phylogenetic tree with 14 tips and 13 internal nodes

Tip labels:
        fuliginosa, fortis, magnirostris, conirostris, scandens, difficilis, ...

Node labels:
        N01, N02, N03, N04, N05, N06, ...

Edge labels:
        E16, E17, E18, E19, E20, E21, ...

Rooted; includes branch lengths
```

Note that the nodes and edges are given default names if the tree contains no node or edge names.

The summary method gives a little extra information, including information on branch lengths:

```
> summary(g1)
 No root edge.
 Phylogenetic tree: g1
 Number of tips
 Number of nodes
                   : 13
 Branch lengths:
                     : 0.1764008
        mean
                     : 0.04624379
        variance
        distribution:
   Min. 1st Qu. Median 3rd Qu.
0.00917 0.04985 0.08000 0.21910 0.88080
  Print tip labels:
> labels(g1)
                                    "magnirostris" "conirostris"
 [1] "fuliginosa"
                    "fortis"
                                                                   "scandens"
                                    "parvulus" "psittacula"
 [6] "difficilis"
                    "pallida"
                                                                   "pauper"
                                    "Pinaroloxias" "olivacea"
[11] "Platyspiza"
                    "fusca"
  Print internal node labels (R automatically assigns values):
> NodeLabels(g1)
 [1] "N01" "N02" "N03" "N04" "N05" "N06" "N07" "N08" "N09" "N10" "N11" "N12"
[13] "N13"
  Print edge labels (also automatically assigned):
> EdgeLabels(g1)
 [1] "E16" "E17" "E18" "E19" "E20" "E21" "E22" "E23" "E24" "E1" "E2" "E3"
[13] "E4" "E5" "E6" "E25" "E7" "E26" "E27" "E8" "E9" "E10" "E11" "E12"
[25] "E13" "E14"
  Is it rooted?
> isRooted(g1)
[1] TRUE
```

Which node is the root?

```
> rootNode(g1)
[1] 15
    Does it have any polytomies?
> hasPoly(g1)
[1] FALSE
    Does it have branch lengths?
> hasEdgeLength(g1)
[1] TRUE
    You can modify labels and other aspects of the tree — for example,
> labels(g1) <- tolower(labels(g1))</pre>
```

You can use plot(g1) to plot the tree (at this point, this just calls the plot.phylo command from the ape package).

Q: what else do people want to do to check their trees?

4 Trees with data

The phylo4d class matches trees with data. (fixme: need to be able to use ioNCL!) or combine it with a data frame to make a phylo4d (tree-with-data) object.

Now we'll take the Geospiza data from geospiza\$geospiza.data and merge it with the tree. However, since G. olivacea is included in the tree but not in the data set, we will initially run into some trouble:

```
> g2 <- phylo4d(g1, geospiza$geospiza.data)
    gives

Error in check_data(res, ...):
    Tip data names are a subset of tree tip labels
(missing data names: platyspiza,pinaroloxias,olivacea)
(extra data names: Pinaroloxias,Platyspiza)</pre>
```

We have two problems — the first is that we forgot to lowercase the labels on the data to match the tip labels:

```
> gdata <- geospiza$geospiza.data
> row.names(gdata) <- tolower(row.names(gdata))</pre>
```

To deal with the second problem (missing data for *G. olivacea*), we have a few choices. The easiest is to use missing.tip.data="OK" to allow R to create the new object:

```
> g2 <- phylo4d(g1, gdata, missing.tip.data = "OK")
```

(setting missing.tip.data to "warn" would create the new object but print a warning).

Another way to deal with this would be to use prune() to drop the offending tip from the tree first:

```
> g1B <- prune(g1, "olivacea")
> phylo4d(g1B, gdata)
```

You can summarize the new object:

> summary(g2)

No root edge.

Phylogenetic tree : as(object, "phylo4")

Number of tips : 14 Number of nodes : 13

Branch lengths:

mean : 0.1764008 variance : 0.04624379

distribution :

Min. 1st Qu. Median 3rd Qu. Max. 0.00917 0.04985 0.08000 0.21910 0.88080

Comparative data:

Tips: data.frame with 14 taxa and 5 variables

wingL	tarsusL	culmenL	beakD
Min. :3.975	Min. :2.807	Min. :1.974	Min. :1.191
1st Qu.:4.189	1st Qu.:2.929	1st Qu.:2.187	1st Qu.:1.941
Median :4.235	Median :2.980	Median :2.311	Median :2.073
Mean :4.236	Mean :2.991	Mean :2.333	Mean :2.083
3rd Qu.:4.265	3rd Qu.:3.039	3rd Qu.:2.430	3rd Qu.:2.347
Max. :4.420	Max. :3.271	Max. :2.725	Max. :2.824
NA's :1.000	NA's :1.000	NA's :1.000	NA's :1.000
gonysW			
Min. :1.401			
1st Qu.:1.845			
Median :1.962			
Mean :2.014			
3rd Qu.:2.222			
Max. :2.676			
NA's :1.000			

Object contains no node data.

Or use tdata() to extract the data (i.e., tdata(g2)). By default, tdata() will retrieve tip data, but you can also get internal node data only (tdata(tree, "node")) or — if the tip and node data have the same format — all the data combined (tdata(tree, "allnode")).

Plotting calls plot.phylog from the ade4 package.

5 Subsetting

The subset command offers a variety of ways of extracting portions of a phylo4 or phylo4d tree, keeping any tip/node data consistent.

tips.include give a vector of tips (names or numbers) to retain

tips.exclude give a vector of tips (names or numbers) to drop

mrca give a vector of node or tip names or numbers; extract the clade containing these taxa

node.subtree give a node (name or number); extract the subtree starting from this node

Different ways to extract the fuliginosa-scandens clade:

```
> subset(g2, tips.include = c("fuliginosa", "fortis", "magnirostris",
+ "conirostris", "scandens"))
> subset(g2, node.subtree = "NO7")
> subset(g2, mrca = c("scandens", "fortis"))

One could drop the clade by doing
> subset(g2, tips.exclude = c("fuliginosa", "fortis", "magnirostris",
+ "conirostris", "scandens"))
> subset(g2, tips.exclude = allDescend(g2, MRCA(g2, c("difficilis",
+ "fortis"))))
```

Another approach is to pick the subtree graphically, by plotting the tree and using identify, which returns the identify of the node you click on with the mouse.

```
> plot(g1)
> n1 <- identify(g1)
> subset(g2, node.subtree = n1)
```

6 Tree-walking

getDescend, getAncest, allDescend, allAncest, getNodeByLabel, getLabelByNode: not sure about the names or functionality of these (how much do we work in terms of labels and how much in terms of internal numbers?)

7 multiPhylo classes

A Definitions/slots

A.1 phylo4

Like ${\tt phylo},$ the main components of the ${\tt phylo4}$ class are:

edge an $N \times 2$ matrix of integers, where the first column ...

edge.length numeric list of edge lengths (length N or empty)

Nnode integer, number of nodes

tip.label character vector of tip labels (required)

node.label character vector of node labels (maybe empty)

root.edge integer defining root edge (maybe NA)

We have defined basic methods for phylo4:show, print (copied from print.phylo inape), and a variety of accessor functions (see help files). summary does not seem to be terribly useful in the context of a "raw" tree, because there is not much to compute: end users?

Print method: add information about (ultrametric, scaled, polytomies (zero-length or structural))?

A.2 phylo4d

The phylo4d class extends phylo4 with data. Tip data, (internal) node data, and edge data are stored separately, but can be retrieved together or separately with tdata(x,"tip") or tdata(x,"all").

edge data can also be included — is this useful/worth keeping?

A.3 multiphylo4

B Validity checking

- number of rows of edge matrix (N) ==length of edge-length vector (if > 0)
- (number of tip labels)+(nNode)-1 == N

- data matrix must have row names
- row names must match tip labels (if not, spit out mismatches)

•

Default node labels:

C Hacks/backward compatibility

Hilmar Lapp very kindly showed a way to hack the \$ operator so that it would provide backward compatibility with code that is extracting internal elements of a phylo4. The basic recipe is:

```
> setMethod("$", "phylo4", function(x, name) {
+    attr(x, name)
+ })
```

but this has to be hacked slightly to intercept calls to elements that might be missing. For example, ape detects whether log-likelihood, root edges, node labels, etc. are missing by testing whether they are NULL, whereas missing items are represented in phylo4 by zero-length vectors in the slots (or NA for the root edge) — so we need code like

```
> if (!hasNodeLabels(x)) NULL else x@node.label
```

to handle these cases.